

Density Dynamics from Current Auto-Correlations at Finite Time- and Length-Scales

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PACS 05.60.Gg – Quantum transport

PACS 05.30.-d – Quantum statistical mechanics

PACS 05.70.Ln – Nonequilibrium and irreversible thermodynamics

Abstract. - We consider the increase of the spatial variance of some inhomogeneous, non-equilibrium density (particles, energy, etc.) in a periodic quantum system of condensed matter-type. This is done for a certain class of initial quantum states which is supported by static linear response and typicality arguments. We directly relate the broadening to some current auto-correlation function at finite times. Our result is not limited to diffusive behavior, however, in that case it yields a generalized Einstein relation. These findings facilitate the approximation of diffusion constants/conductivities on the basis of current auto-correlation functions at finite times for finite systems. Pursuing this, we quantitatively confirm the magnetization diffusion constant in a spin chain which was recently found from non-equilibrium bath scenarios.

Any current of some physical quantity like, e.g., electrons through solids is either induced by an external mechanical force \mathbf{F} (e.g., electric field) or a spatially non-uniform density (density gradient $\nabla\rho$). For systems featuring normal transport the currents in those two cases are routinely assumed to be determined by

$$\mathbf{j} = \kappa \mathbf{F}, \quad \mathbf{j} = -\mathcal{D} \nabla \rho, \quad (1)$$

where \mathbf{j} denotes the current; κ the conductivity; and \mathcal{D} the diffusion constant. As well-known, the derivation of the l.h.s. of Eq. (1) from linear response theory is rather straightforward and leads to the Kubo formula [1] which nowadays is a standard approach to transport in quantum systems [2–7]. However, a direct derivation of the r.h.s. of Eq. (1) from the corresponding scenario, i.e., without any external force appears to be more subtle. The overview paper [8] by Zwanzig, e.g., lists essentially six families of approaches, each of them based on different sorts of assumptions such as Fokker-Planck dynamics in the space of relevant observables [9–11], Onsager’s regression hypothesis [12,13], restriction of the dynamics to local equilibrium states [14], etc. These subtleties are especially disturbing in the context of heat conduction, since there simply is no practical external force which could cause a heat cur-

rent [15–19]. However, all of the above approaches eventually give the diffusion constant in terms of current auto-correlation functions also, i.e., proportional to the conductivity. Of course, this is what Einstein and Smolouchowski firstly suggested in their ground-breaking work on Brownian motion. The above approaches are comprehensively covered in textbooks like, e.g., [1]. Therein the interested reader may also find a discussion of their consistency and implications. In order to motivate our present alternative approach to this extensively debated subject, we simply discuss here a standard formulation rather than going through the above discussion. In [1], e.g., one finds the following expression for a particle diffusion coefficient

$$\mathcal{D} = \frac{1}{kT\partial n/\partial\xi} \lim_{\omega\rightarrow 0} \int_0^\infty dt e^{i\omega t} \lim_{\substack{q\rightarrow 0 \\ L\rightarrow\infty}} \frac{\langle J'_{-q}(0); J'_q(t) \rangle}{L^3}, \quad (2)$$

where n is the equilibrium particle density; ξ the chemical potential; J' denotes the “random current”; J'_q its Fourier component with wavevector q ; the brackets encode the Kubo-inner product; and L^3 is the volume of the system. Conceptually, the most challenging part is probably to concisely show that in the above limit the auto-correlation of the random current may be replaced by the auto-correlation of the “true current”, i.e., $\langle J'_{-q}(0); J'_q(t) \rangle \rightarrow \langle J_{-q}(0); J_q(t) \rangle$ (since the former involves the “irrelevant part” in terms of projection meth-

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ods), however, this replacement appears to be generally accepted. Practically, the limits $q \rightarrow 0$, $\omega \rightarrow 0$ imply that only the infinitely slow dynamics of density structures of infinite length scale can be expected to behave diffusively with the above diffusion coefficient. So, even if one knew the exact current auto-correlation function for the infinite system, that would not bare implications on the dynamics at finite time- or length-scales. And, even worth, if one has some information on the current auto-correlation function but only up to a finite time, (2) does not allow for any conclusions on the dynamics. Both issues become manifest, if the integral in (2) does not converge, then no information results except for the “non-diffusiveness” of the dynamics. Furthermore, it may be a little subtle to generalize (2) to, e.g., a micro canonical ensemble.

Thus, in this paper we approach the subject neither from projection techniques nor from linear response. Instead we (somewhat arbitrarily) “coarse-grain” the quantum system spatially into subunits. The density profile and the current operator are then discretely formulated on the basis of this coarse-grained description. Afterwards a specific class of initial states featuring such a non-uniform density profile is introduced. Then, simply by applying Heisenberg’s equation, the evolution of the variance of the density profile is expressed in terms of a double temporal integral of the current auto-correlation function. Based on this result, we discuss the connection between diffusion coefficient and conductivity. We further discuss the implications of our specific choice for the initial state w.r.t. external perturbations and quantum typicality. Finally, we numerically calculate the integral of the magnetization current auto-correlation function in a XXZ spin chain and quantitatively compare the outcome to recent results on the diffusion constants for such a system from non-equilibrium bath scenarios.

The above mentioned periodic spatial coarse-graining scheme is introduced to facilitate a consistent definition of a local current. It is most conveniently explained for (but not limited to) an one-dimensional system. To those ends the transported quantity \hat{X} as well as the Hamiltonian \hat{H} are decomposed into formally identical addends which correspond to different positions, i.e., $\sum_{\mu} \hat{x}_{\mu} = \hat{X}$, $\sum_{\mu} \hat{h}_{\mu} = \hat{H}$. Thus, \hat{x}_{μ} is a local density of the transported quantity. Note that the \hat{h}_{μ} may be defined on or in between the positions of the \hat{x}_{μ} , or both. We consider quantities which are conserved on the full system, i.e., $[\hat{H}, \hat{X}] = 0$. We further require

$$\dot{\hat{x}}_{\mu} = i[\hat{H}, \hat{x}_{\mu}] = \underbrace{i[\hat{h}_{\mu-}, \hat{x}_{\mu}]}_{\equiv \hat{j}_{\mu-1}} + \underbrace{i[\hat{h}_{\mu+}, \hat{x}_{\mu}]}_{\equiv -\hat{j}_{\mu}}. \quad (3)$$

Here, $\hat{h}_{\mu-}$ ($\hat{h}_{\mu+}$) is supposed to denote the local subunit of the Hamiltonian which is located directly on the l.h.s. (r.h.s.) of \hat{x}_{μ} . This implies a kind of locality. However, such a description may always be at least approximately enforced, if the interactions are reasonably short-

ranged. It may require the usage of \hat{h}_{μ} that are larger than a single elementary cell. Routinely, the comparison with a continuity equation suggests a definition of local currents according to the scheme indicated in Eq. (3) [2, 3, 6, 20]. This is consistent, if $[\hat{h}_{\mu+}, \hat{x}_{\mu}] + [\hat{h}_{(\mu+1)-}, \hat{x}_{(\mu+1)}] = 0$. The latter holds, if \hat{X} is globally conserved.

We now define the class of initial states we are going to consider. Those read

$$\rho(0) \equiv \rho_{\text{eq}} + \sum_{\mu} \frac{\delta_{\mu}}{\epsilon^2} \rho_{\text{eq}}^{\frac{1}{2}} \hat{d}_{\mu} \rho_{\text{eq}}^{\frac{1}{2}}, \quad \hat{d}_{\mu} \equiv \hat{x}_{\mu} - \langle \hat{x}_{\mu} \rangle. \quad (4)$$

Here, ρ_{eq} is any stationary (equilibrium) state of the full system, i.e., $[\hat{H}, \rho_{\text{eq}}] = 0$. The brackets $\langle \dots \rangle$ denote full equilibrium averages, i.e., $\langle \hat{A} \rangle \equiv \text{Tr}\{\hat{A} \rho_{\text{eq}}\}$. Let $\langle\langle \hat{A}; \hat{B} \rangle\rangle$ indicate the inner product $\langle\langle \hat{A}; \hat{B} \rangle\rangle \equiv \text{Tr}\{\hat{A} \rho_{\text{eq}}^{\frac{1}{2}} \hat{B} \rho_{\text{eq}}^{\frac{1}{2}}\}$. We then define

$$c(t, \mu - \nu) \equiv \frac{1}{\epsilon^2} \langle\langle \hat{d}_{\mu}(t); \hat{d}_{\nu} \rangle\rangle, \quad \epsilon^2 \equiv \sum_{\mu} \langle\langle \hat{d}_{\mu}(t); \hat{d}_{\nu} \rangle\rangle \quad (5)$$

which clarifies the ϵ^2 from (4). ϵ^2 does not depend on time, for periodic systems it further does not depend on ν . For interpretational reasons we note that in this case ϵ^2 may be rewritten as $\epsilon^2 = \langle\langle \hat{X} - \langle \hat{X} \rangle; \hat{X} - \langle \hat{X} \rangle \rangle\rangle / L = \langle (\hat{X} - \langle \hat{X} \rangle)^2 \rangle / L$ (here we exploited $[\hat{X}, \hat{H}] = 0$), where now and in the following L indicates the number of subunits in the full system. ϵ^2 hence quantifies the equilibrium fluctuations of the transported quantity. Thus, w.r.t. (2), this implies $\epsilon^2 = kT \partial n / \partial \xi$.

We denote the actual expectation value of the local deviation of the transported quantity from full equilibrium by $d_{\mu}(t)$, i.e.,

$$d_{\mu}(t) \equiv \text{Tr}\{\hat{d}_{\mu}(t) \rho(0)\}. \quad (6)$$

This way we may write

$$d_{\mu}(t) = \sum_{\nu} c(t, \mu - \nu) \delta_{\nu}, \quad \text{thus} \quad \sum_{\mu} d_{\mu}(t) = \sum_{\mu} \delta_{\mu}. \quad (7)$$

We are going to analyze the spatial variance of those deviations from equilibrium, while we require them to be normalized to one, i.e., $\sum_{\mu} d_{\mu}(0) = 1$. The normalization is implemented by a corresponding choice of the δ_{μ} . Then we may directly, quantitatively compare to a discrete diffusion equation, as outlined below. The above mentioned spatial variance $W^2(t)$ simply reads

$$W^2(t) \equiv \sum_{\mu} \mu^2 d_{\mu}(t) - \left[\sum_{\mu} \mu d_{\mu}(t) \right]^2. \quad (8)$$

If now, hypothetically, the dynamics of the $d_{\mu}(t)$ were generated by a discrete diffusion equation of the form

$$\dot{d}_{\mu}(t) = \mathcal{D}(t) [d_{\mu-1}(t) - 2d_{\mu}(t) + d_{\mu+1}(t)], \quad (9)$$

then the evolution of the variance would read

$$[\dot{W}^2](t) \approx 2\mathcal{D}(t) \quad (10)$$

which holds, if the $d_\mu(t)$ vanish at the ends of a chain or are reasonably concentrated at a sector of a ring. (Such a concentration will be assumed throughout this paper.) Exploiting this, we are able to deduce a diffusion constant $\mathcal{D}(t)$ from the evolution of the variance. To those ends we rewrite the variance using (7) which yields

$$W^2(t) = \sum_\mu \mu^2 \delta_\mu + \sum_\eta \eta^2 c(t, \eta) - \left[\sum_\mu \mu \delta_\mu \right]^2 - \left[\sum_\eta \eta c(t, \eta) \right]^2. \quad (11)$$

If the system features “space inversion symmetry”, which we assume in the following, the last term on the r.h.s. of the above Eq. (11) vanishes. In order to relate the evolution of $W^2(t)$ to a current auto-correlation function, it turns out to be helpful to consider its second derivative w.r.t time. According to (11), this reads

$$[\ddot{W}^2](t) = \sum_\eta \eta^2 \ddot{c}(t, \eta). \quad (12)$$

We may evaluate this using Heisenberg’s equation:

$$\ddot{c}(t, \eta) = -\frac{1}{\epsilon^2} \langle [\hat{H}, [\hat{H}, \hat{d}_\eta(t)]]; \hat{d}_0 \rangle \quad (13)$$

which may be rewritten as

$$\ddot{c}(t, \eta) = -\frac{1}{\epsilon^2} \langle \imath [\hat{H}, \hat{d}_\eta(t)]; \imath [\hat{H}, \hat{d}_0] \rangle \quad (14)$$

or, exploiting (3) and (4), as

$$\ddot{c}(t, \eta) = -\frac{1}{\epsilon^2} \langle (\hat{j}_{\eta-1} - \hat{j}_\eta); (\hat{j}_{-1} - \hat{j}_0) \rangle. \quad (15)$$

Inserting the above Eq. (15) into (12), and exploiting again that $\langle \hat{j}_{\eta+\zeta}(t); \hat{j}_\eta \rangle$ does not depend on η and further vanishes for $\zeta \rightarrow L$, we obtain

$$[\ddot{W}^2](t) = \frac{2}{L \epsilon^2} \langle \hat{J}(t); \hat{J} \rangle. \quad (16)$$

Here, \hat{J} denotes not a local but the total current in the full system, i.e., $\hat{J} \equiv \sum_\mu \hat{j}_\mu$. According to (10), the diffusion constant corresponds to the first derivative of the variance which reads

$$[\dot{W}^2](t) = [\dot{W}^2](t=0) + 2 \int_0^t dt' \frac{1}{L \epsilon^2} \langle \hat{J}(t'); \hat{J} \rangle. \quad (17)$$

We suggest here to assume that $[\dot{W}^2](t=0) = 0$. This surely holds for $T \rightarrow \infty$, since in that limit $W^2(t)$ is symmetric w.r.t. time. However, irrespective of T , according to typicality arguments, there are overwhelmingly more (pure) states corresponding to higher W^2 compared to any lower W^2 [21]. Thus, it is not to be expected that any state evolves towards lower W^2 , forwards or backwards in time, unless it has been deliberately constructed

to do so. We hence expect $W^2(t)$ to be essentially symmetric w.r.t. time, irrespective of T . Comparing to (10), we eventually conclude for the diffusion constant

$$\mathcal{D}(t) = \int_0^t dt' \frac{1}{L \epsilon^2} \langle \hat{J}(t'); \hat{J} \rangle, \quad (18)$$

which is the first main result of this work.

In order to compare this to force-driven transport (as calculated from the Kubo formula), we write out the integrand in (18) explicitly finding

$$\frac{1}{L \epsilon^2} \langle \hat{J}(t); \hat{J} \rangle = \frac{1}{L \epsilon^2} \sum_{m,n} (p_m p_n)^{\frac{1}{2}} \|J_{mn}\|^2 \cos(\omega_{mn} t) \quad (19)$$

with $p_m \equiv (\rho_{\text{eq}})_{mm}$, J_{mn} as the matrix elements of the respective operators in the energy eigenbasis and with $\omega_{mn} = E_m - E_n$ as the difference of the energy eigenvalues E_m, E_n . Force-driven transport (within the linear regime) is routinely described by a response function that relates the current density to the external force:

$$j(t) = \int_{-\infty}^t dt' \Phi(t') F(t'). \quad (20)$$

For a canonical equilibrium the low-frequency part of $\Phi(t)$, for which $\omega_{mn} \ll kT$ applies, may be written as

$$\Phi^{\text{low}}(t) = \frac{1}{L kT} \sum_{m,n} (p_m p_n)^{\frac{1}{2}} \|J_{mn}\|^2 \cos(\omega_{mn} t). \quad (21)$$

Thus, defining the response to slowly varying fields as $\sigma(t) \equiv \int_0^t dt' \Phi(t')$, we get for times $t \gg \hbar/kT$

$$\mathcal{D}(t) = \frac{kT}{\epsilon^2} \sigma(t) \quad (22)$$

which is a somewhat generalized Einstein relation, since it applies to all quantities (not only particles). Obviously, in the case of diffusive transport the time dependencies of $\mathcal{D}(t)$ and $\sigma(t)$ are expected to vanish.

In the following we will discuss the choice of the initial non-equilibrium state in Eq. (4). This choice is essentially supported by two arguments.

(I.) Assume the system was exposed (before any transport dynamics starts) to an, additionally weak, static “potential” such that the perturbed Hamiltonian reads $\hat{H}' = \hat{H} + \sum_\mu v_\mu \hat{x}_\mu$. Then the corresponding canonical equilibrium state surely is given by $\rho'_{\text{eq}} = \exp(-\hat{H}'/kT)/\text{Tr}\{\exp(-\hat{H}'/kT)\}$. (Note that this is of the same form as a so-called “local equilibrium state”). Now, ρ'_{eq} may be calculated for small v_μ using static linear response [1]. Doing so, one finds that “low-frequency” contributions of the “non-homogeneous” parts of ρ'_{eq} and $\rho(0)$ are proportional to each other, i.e.,

$$(\rho'_{\text{eq}} - \rho_{\text{eq}})_{mn} \propto (\rho(0) - \rho_{\text{eq}})_{mn} \quad \text{for } |\omega_{mn}| \ll kT, v_\mu \propto \delta_\mu \quad (23)$$

with ρ_{eq} as the canonical state w.r.t. to \hat{H} alone. All the dynamics of ρ'_{eq} and $\rho(0)$ under \hat{H} stem from their inhomogeneous parts. All dynamics for times $t \gg \hbar/kT$ is controlled by their low-frequency contributions. In other words: if the initial density profile is induced by a previous static external potential (which is then removed), the broadening of this density profile can be expected to be of the same form as the broadening corresponding to the hypothetical initial state $\rho(0)$, as discussed in detail above. Our considerations therefore apply to this frequently discussed type of initial state.

(II.) A possibly even stronger motivation for the consideration of the initial states in Eq. (4) may be given along the lines of typicality [21–23]. Recently, it has been pointed out that in quantum systems with large Hilbert space dimensions the evolutions of observables of the type $\langle \psi(t) | \hat{A} | \psi(t) \rangle$ do not depend crucially on the details of the initial state $|\psi(0)\rangle$ [24]. Concretely, this means that the overwhelming majority of a set of initial states $|\psi_n(0)\rangle$ which all feature the same initial expectation value a of an observable \hat{A} , i.e. $\langle \psi_n(0) | \hat{A} | \psi_n(0) \rangle = a$, will approximately yield the same evolution of this expectation value, namely $\langle \psi_n(t) | \hat{A} | \psi_n(t) \rangle \approx \text{Tr}\{\hat{A} \rho^{\text{HE}}(t)\}$, where $\rho^{\text{HE}}(t)$ represents a Hilbert space ensemble and explicitly reads $\rho^{\text{HE}}(0) = 1 + f\hat{A}$, where $f = f(a)$ is a pertinent scalar function of a . Although not proven so far, it is natural to suggest a generalization of this dynamical typicality to many observables such that for an initial set specified by $\langle \psi_n(0) | \hat{A}_m | \psi_n(0) \rangle = a_m$ there exist typical evolutions for the expectation values of the type $\langle \psi_n(t) | \hat{A}_m | \psi_n(t) \rangle \approx \text{Tr}\{\hat{A}_m \rho^{\text{HE}}(t)\}$ but now with a $\rho^{\text{HE}}(0) = 1 + \sum_m f_m \hat{A}_m$, where the $f_m = f_m(\{a_l\})$ are functions of the a_l . If we consider for the moment a micro canonical ensemble in (4), we have to choose $\rho_{\text{eq}} = \hat{\Pi}_E / \text{Tr}\{\hat{\Pi}_E\}$ with $\hat{\Pi}_E$ being a projector projecting out the subspace spanned by the energy eigenstates corresponding to energies within a certain interval around E . With this choice the initial state in (4) reads $\rho(0) = \hat{\Pi}_E (1 + \sum_\mu \delta_\mu / \epsilon^2 \hat{d}_\mu) \hat{\Pi}_E / \text{Tr}\{\hat{\Pi}_E\}$ which essentially is the same state as the latter $\rho^{\text{HE}}(0)$ with $\hat{A}_\mu = \hat{d}_\mu$ within the respective subspace. Thus, even if the true physical initial state may not be of the precise form in (4), the initial state in (4) nevertheless generates the typical evolution of the spatial density profile. Or to rephrase, if some initial state features a given spatial density profile and lives within a given energy region, the dynamical broadening of the density profile will most likely be described by (17), irrespective of the details of the initial state.

Finally, we compare approximations to the diffusion constant $\mathcal{D}(t)$, as given by Eq. (18), with recent results in the literature. We approximate $\mathcal{D}(t)$ for finite times, simply by numerically exact diagonalization of finite systems. Concretely, we analyze magnetization transport, i.e. $\hat{x}_\mu = \hat{\sigma}_\mu^z / 2$, in the anisotropic $s = 1/2$ Heisenberg

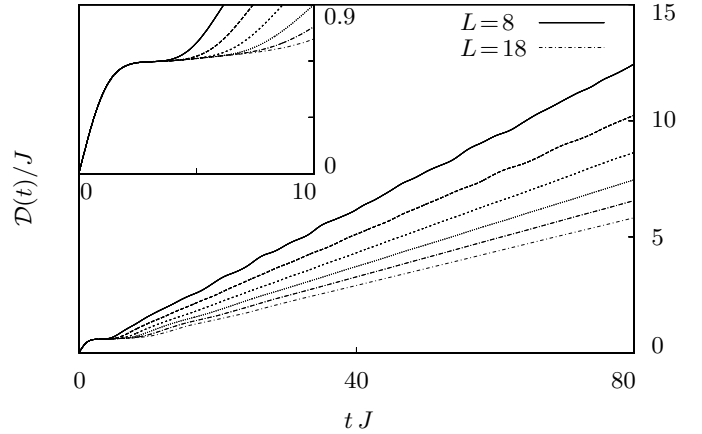


Fig. 1: The diffusion constant $\mathcal{D}(t)$, as defined by Eq. (18), for magnetization transport (spin transport) in the anisotropic $s = 1/2$ Heisenberg chain (XXZ model) in the limit of high temperatures ($\beta = 0$), evaluated numerically (exact diagonalization) for chain lengths $L = 8, 10, \dots, 18$. The curves for $\mathcal{D}(t)$ correspond to the anisotropy parameter $\Delta = 1.5$ and are independent from the concrete choice of the field strength B .

chain (XXZ chain) with periodic boundary conditions:

$$\hat{H} = \sum_{\mu=1}^L \frac{J}{4} (\hat{\sigma}_\mu^x \hat{\sigma}_{\mu+1}^x + \hat{\sigma}_\mu^y \hat{\sigma}_{\mu+1}^y + \Delta \hat{\sigma}_\mu^z \hat{\sigma}_{\mu+1}^z) + \frac{B}{2} \hat{\sigma}_\mu^z. \quad (24)$$

Here, the operators $\hat{\sigma}_\mu^i$ ($i = x, y, z$) represent the standard Pauli matrices (corresponding to site μ); J denotes the coupling strength; Δ is the anisotropy parameter; and B specifies the strength of the magnetic field.

Fig. 1 exemplarily shows the result for $\Delta = 1.5$ and $\beta = 0$ for various lengths $L = 8, 10, \dots, 18$. Note that in this high temperature regime the results are independent from B . At short times (inset) we find an approximately constant $\mathcal{D}(t) \approx \mathcal{D} = 0.6 J$. While the height of this “plateau” does not change with L , its width seems to increase gradually. This increase is plausible, especially since the slope of $\mathcal{D}(t)$ at large t coincides with the Drude weight and is expected to vanish in the limit of $L \rightarrow \infty$ [2, 3, 6]. Remarkably, $\mathcal{D} = 2.4$ for $J = 4$ is very close to the value of 2.3 which was found in Ref. [25] from a numerically involved analysis of a bath scenario. Furthermore, for a slightly different anisotropy $\Delta = 1.6$ a similar Fig. with $\mathcal{D} = 0.55 J$ is found, i.e., $\mathcal{D} = 0.022$ for $J = 0.04$. Also this result is in very good agreement with the value of 0.0234 in Ref. [26] which also addresses the high temperature limit using bath scenarios.

These numerical findings support the typicality statement, i.e., that the range of validity of (18) is not limited to the specific scenario, as explicitly analyzed in the text. Thus, in a forthcoming paper [27] by two of us Eq. (18) will be applied to various spin models in detail.

We sincerely thank F. Heidrich-Meisner for fruitful dis-

cussions. Financial support by the Deutsche Forschungsgemeinschaft is gratefully acknowledged.

REFERENCES

- [1] R. KUBO, M. YOKOTA and S. HASHTISUME, *Statistical Physics II: Nonequilibrium Statistical Mechanics* 2nd Edition Vol. 31 of *Solid State Sciences* (Springer) 1991.
- [2] X. ZOTOS, *Phys. Rev. Lett.* , **82** (1999) 1764.
- [3] F. HEIDRICH-MEISNER, A. HONECKER, D. C. CABRA and W. BRENIG, *Phys. Rev. B* , **68** (2003) 134436.
- [4] K. SAITO, *Europhys. Lett.* , **61** (2003) 34.
- [5] X. ZOTOS and P. PRELOVSEK, *Interacting Electrons in Low Dimensions* Vol. 25 of *Physics and Chemistry of Materials with Low-Dimensional Structures* (Kluwer Academic Publishers) 2003 Ch. Transport in One-Dimensional Quantum Systems.
- [6] J. BENZ, T. FUKUI, A. KLÜMPER and C. SCHEEREN, *J. Phys. Soc. Jpn. Suppl.* , **74** (2005) 181.
- [7] C. MEJÍA-MONASTERIO, T. PROSEN and G. CASATI, *Europhys. Lett.* , **72** (2005) 520.
- [8] R. ZWANZIG, *Annu. Rev. Phys. Chem.* , **16** (1965) 67.
- [9] J. G. KIRKWOOD, *J. Chem. Phys.* , **14** (1946) 180.
- [10] M. S. GREEN, *J. Chem. Phys.* , **20** (1952) 1281.
- [11] S. R. DEGROOT and P. MAZUR, *Non-Equilibrium Thermodynamics* (North-Holland, Amsterdam) 1962.
- [12] L. ONSAGER, *Phys. Rev.* , **37** (1931) 405.
- [13] R. KUBO, M. YOKOTA and S. NAKAJIMA, *J. Phys. Soc. Jpn.* , **12** (1957) 1203.
- [14] H. MORI, *Phys. Rev.* , **112** (1958) 1829.
- [15] J. M. LUTTINGER, *Phys. Rev.* , **135** (1964) A1505.
- [16] P. L. GARRIDO, P. I. HURTADO and B. NADROWSKI, *Phys. Rev. Lett.* , **86** (2001) 5486.
- [17] K. SAITO and S. MAYASHITA, *J. Phys. Soc. Jpn.* , **71** (2002) 2485.
- [18] S. LEPRI, R. LIVI and A. POLITI, *Physics Reports* , **377** (2003) 1.
- [19] L.-A. WU and D. SEGAL, *Phys. Rev. E* , **77** (2008) 060101(R).
- [20] J. GEMMER, R. STEINIGEWEG and M. MICHEL, *Phys. Rev. B* , **73** (2006) 104302.
- [21] P. REIMANN, *Phys. Rev. Lett.* , **99** (2007) 160404.
- [22] S. GOLDSTEIN, J. L. LEBOWITZ, R. TUMULKA and N. ZANGHI, *Phys. Rev. Lett.* , **96** (2006) 050403.
- [23] S. POPESCU, A. J. SHORT and A. WINTER, *Nature Phys.* , **2** (2006) 754.
- [24] C. BARTSCH and J. GEMMER, *Phys. Rev. Lett.* , **102** (2009) 110403.
- [25] T. PROSEN and M. ŽNIDARIČ, *J. Stat. Mech.* , **2009** (2009) P02035.
- [26] M. MICHEL, O. HESS, H. WICHTERICH and J. GEMMER, *Phys. Rev. B* , **77** (2008) 104303.
- [27] R. STEINIGEWEG, and J. GEMMER, *arXiv:0906.4457*, (2009) .